

L Number	Hits	Search Text	DB	Time stamp
1	52223	Grignard reagent and Magnesium	USPAT	2003/11/21 09:18
2	37061	Grignard reagent and Lithium	USPAT	2003/11/21 09:19
3	30187	(Grignard reagent and Magnesium) and (Grignard reagent and Lithium)	USPAT	2003/11/21 09:19
4	607817	((Grignard reagent and Magnesium) and (Grignard reagent and Lithium)) and boronic acid	USPAT	2003/11/21 09:19
5	607817	((Grignard reagent and Magnesium) and (Grignard reagent and Lithium)) and borinic acid	USPAT	2003/11/21 09:20
6	608349	((Grignard reagent and Magnesium) and (Grignard reagent and Lithium)) and phenyl boronic acid	USPAT	2003/11/21 09:20
7	608384	((Grignard reagent and Magnesium) and (Grignard reagent and Lithium)) and aryl boronic acid	USPAT	2003/11/21 09:21
8	37184	ary halide and Lithium	USPAT	2003/11/21 09:21
9	156554	Aryl halide and Lithium	USPAT	2003/11/21 09:21
10	257	Fluoropheny and lithium	USPAT	2003/11/21 09:23
11	607817	(Fluoropheny and lithium) and boronic acid	USPAT	2003/11/21 09:22
12	607817	(Fluoropheny and lithium) and borinic acid	USPAT	2003/11/21 09:22
13	9409	Fluoropheny and lithium	USPAT	2003/11/21 09:24
14	251	(Fluoropheny and lithium) and (Fluoropheny and lithium)	USPAT	2003/11/21 09:25
15	6679	Fluoropheny and lithium and synthesis	USPAT	2003/11/21 09:25
16	5252	(Fluoropheny and lithium and synthesis) and process	USPAT	2003/11/21 09:25
17	249662	((Fluoropheny and lithium and synthesis) and process) and one pot synthesis	USPAT	2003/11/21 09:26
18	1168461	(Fluoropheny and lithium and synthesis) and process) and one step	USPAT	2003/11/21 09:27
19	55157	((Fluoropheny and lithium and synthesis) and process) and one pot	USPAT	2003/11/21 09:27

Welcome to STN International! Enter x:x

LOGINID:sssptal611sxp

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1	Web Page URLs for STN Seminar Schedule - N. America
NEWS 2	"Ask CAS" for self-help around the clock
NEWS 3 SEP 09	CA/CAPplus records now contain indexing from 1907 to the present
NEWS 4 AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS 5 AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 6 AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS 7 AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS 8 AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS 9 AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS 10 SEP 22	DIPPR file reloaded
NEWS 11 SEP 25	INPADOC: Legal Status data to be reloaded
NEWS 12 SEP 29	DISSABS now available on STN
NEWS 13 OCT 10	PCTFULL: Two new display fields added
NEWS 14 OCT 21	BIOSIS file reloaded and enhanced
NEWS 15 OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS EXPRESS	NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:42:40 ON 21 NOV 2003

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

Patel

<11/20/2003>

FILE 'CAPLUS' ENTERED AT 11:42:50 ON 21 NOV 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Nov 2003 VOL 139 ISS 22
FILE LAST UPDATED: 20 Nov 2003 (20031120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s lithium and organo compounds
L1 0 LITHIUM AND ORGANO COMPOUNDS

=> s phenyl lithium and halide
L2 30 PHENYL LITHIUM AND HALIDE

=> s l2 and sy nthesis
L3 0 L2 AND SY NTHESIS

=> s l2 and synthesis
L4 6 L2 AND SYNTHESIS

=> s phenyl boro nic acids and synthesis
L5 0 PHENYL BORO NIC ACIDS AND SYNTHESIS

=> s phenyl boronic acids and process
L6 0 PHENYL BORONIC ACIDS AND PROCESS

=> s phenyl boronic acids and making
L7 0 PHENYL BORONIC ACIDS AND MAKING

=> s l2 and phenyl boronic acid
L8 0 L2 AND PHENYL BORONIC ACID

=> d l4 fbib hitstr abs total

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:163600 CAPLUS
DN 130:296803
TI Models for the initial stages of oxidative addition. **Synthesis**, characterization, and mechanistic investigation of .eta.1-I2 organometallic "pincer" complexes of platinum. X-ray crystal structures of [PtI(C6H3[CH2NMe2])2-2,6](.eta.1-I2)] and exo-meso-[Pt(.eta.1-I3)(.eta.1-I2)(C6H3[CH2N(t-Bu)Me])2-2,6)]

AU Gossage, Robert A.; Ryabov, Alexander D.; Spek, Anthony L.; Stufkens, Derk J.; van Beek, Johannes A. M.; van Eldik, Rudi; van Koten, Gerard
CS Department of Metal-Mediated Synthesis Debye Institute and Laboratory of Crystal Chemistry, Bijvoet Center for Biomolecular Research, Utrecht University, Utrecht, 3584 CH, Neth.
SO Journal of the American Chemical Society (1999), 121(11), 2488-2497
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The reaction of I₂ with Pt pincer complexes [PtI(NCN'')] (NCN'' = [C₆H₃(CH₂NRR')₂-2,6]-; R = R' = Me or Et; or R = Me, R' = t-Bu) is reported. All three complexes contain an end-on (.eta.1) I₂ unit, and these compds. represent the only known isolable organometallic species which contain I₂ in this bonding motif. These compds. can be envisioned as representing the initial stages of oxidative addn. of dihalides to d⁸ transition metal complexes. [PtI{C₆H₃(CH₂NMe₂)₂-2,6}(.eta.1-I₂)] (1) and exo-meso-[PtI₃{C₆H₃(CH₂NMe[t-Bu])₂-2,6}(.eta.1-I₂)] (3b) were structurally characterized by single-crystal x-ray diffraction methods. Mechanistic and spectroscopic (IR, Raman, NMR, UV/visible) studies indicated that complex 1 is formed via a 1,2-shift of the dihalide from the primary product [Pt(.eta.1-I₃){C₆H₃(CH₂NMe₂)₂-2,6}]. The role of the metal-bound **halide** anion as the point of initial attack of I₂ is described. The results of these studies are discussed in terms of the basic mechanism of oxidative addn. and its implications for catalysis.
RE.CNT 164 THERE ARE 164 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:347170 CAPLUS
DN 127:17742
TI **Synthesis** and Structures of Intramolecularly Base-Coordinated Group 15 Aryl **Halides**
AU Carmalt, Claire J.; Cowley, Alan H.; Culp, Robert D.; Jones, Richard A.; Kamepalli, Smuruthi; Norman, Nicholas C.
CS Department of Chemistry Biochemistry, University of Texas, Austin, TX, 78712, USA
SO Inorganic Chemistry (1997), 36(13), 2770-2776
CODEN: INOCAJ; ISSN: 0020-1669
PB American Chemical Society
DT Journal
LA English
AB Four group 15 monochlorides of the type EAr₂Cl [Ar = 2-[(dimethylamino)methyl]phenyl, 2-(Me₂NCH₂)C₆H₄ (C₉H₁₂N), E = Sb (4), E = Bi (5); Ar = 8-(dimethylamino)-1-naphthyl, 8-(Me₂N)C₁₀H₆ (C₁₂H₁₂N), E = Sb (6), E = Bi (7)] have been prepd. via the salt elimination reactions of 2 equiv. of either 2-(Me₂NCH₂)C₆H₄Li or 8-(Me₂N)C₁₀H₆Li with ECl₃. Four related group 15 dihalides of the type EArX₂ [Ar = 8-(Me₂N)C₁₀H₆, X = Cl, E = As, (8), E = Sb (9); Ar = 2-(Me₂NCH₂)C₆H₄, X = Cl, E = Bi (10); X = I, E = Bi (11)] have been prepd. via the salt elimination reactions of equimolar amts. of 8-(Me₂N)C₁₀H₆Li or 2-(Me₂NCH₂)C₆H₄Li with EX₃. The x-ray crystal structures of 4-6, 8, 9, and 11 are described, and the obsd. trends in the degree of intramol. coordination of the nitrogen atoms are consistent with the view that the Lewis acidity of these complexes is assocd. with the E-X .sigma.* orbitals. Crystal data for 4: triclinic, space group P.hivin.1, a = 9.1483(1) .ANG., b = 9.4868(1) .ANG., c = 12.9776(2) .ANG., .alpha. = 70.614(8).degree., .beta. = 85.738(9).degree., .gamma. = 83.094(9).degree., V = 1054.0(2) .ANG.³, Z = 2, R = 0.0420.

Crystal data for 5: monoclinic, space group P21/c, a = 11.9498(1) .ANG., b = 11.4695(1) .ANG., c = 13.9456(8) .ANG., .beta. = 104.536(6).degree., V = 1850.2(3) .ANG.³, Z = 4, R = 0.0375. Crystal data for 6: monoclinic, space group P21/n, a = 9.4991(8) .ANG., b = 23.455(4) .ANG., c = 9.726(1) .ANG., .beta. = 100.629(8).degree., V = 2129.8(4) .ANG.³, Z = 4, R = 0.0406. Crystal data for 8: orthorhombic, space group P212121, a = 9.713(3) .ANG., b = 9.835(4) .ANG., c = 13.310(3) .ANG., V = 1273.8(5) .ANG.³, Z = 4, R = 0.0695. Crystal data for 9: orthorhombic, space group P212121, a = 9.7140(3) .ANG., b = 10.0196(1) .ANG., c = 13.444(3) .ANG., V = 1308.5(3) .ANG.³, Z = 4, R = 0.0320. Crystal data for 11: monoclinic, space group P21/c, a = 7.9455(7) .ANG., b = 19.3949(3) .ANG., c = 8.6226(9) .ANG., .beta. = 93.338(9).degree., V = 1326.5(2) .ANG.³, Z = 4, R = 0.0379.

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1997:286305 CAPLUS

DN 126:251198

TI **Synthesis** and Characterization of the Monomeric Diaryls

M{C6H3-2,6-Mes2}2 (M = Ge, Sn, or Pb; Mes = 2,4,6-Me3C6H2-) and Dimeric Aryl-Metal Chlorides [M(Cl){C6H3-2,6-Mes2}]2 (M = Ge or Sn)

AU Simons, Richard S.; Pu, Lihung; Olmstead, Marilyn M.; Power, Philip P.

CS Department of Chemistry, University of California, Davis, CA, 95616, USA

SO Organometallics (1997), 16(9), 1920-1925

CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

OS CASREACT 126:251198

AB The reaction of 2 equiv of LiC6H3-2,6-Mes2 (Mes = 2,4,6-Me3C6H2) with GeCl2.cntdot.dioxane, SnCl2, or PbCl2 in ether soln. gave rare examples of monomeric, .sigma.-bonded, diaryl derivs. M{C6H3-2,6-Mes2}2 (M = Ge (1), Sn (2), or Pb (3)). The compds. 1-3 are thermally stable, purple, cryst. solids with V-shaped geometries and remarkably wide (.apprx.114.5.degree.) interligand bond angles. The monoaryl metal chloride derivs. [M(Cl){C6H3-2,6-Mes2}]2 (M = Ge (4) or Sn (5)) were isolated by treatment of the appropriate dichlorides with either 1 equiv of LiC6H3-2,6-Mes2 or 1 equiv of the diaryls 1 or 2. The orange Ge compd. 4 has a dimeric structure in which the monomers are linked by a relatively weak, 2.443(2) .ANG., Ge-Ge interaction. In sharp contrast, its yellow Sn analog 5 has a dimeric structure in which three-coordinate Sn centers are assocd. by asym. bridging chlorides. The compds. 1-3 constitute a unique, structurally characterized diaryl series for Ge, Sn, and Pb and display evidence of steric crowding that is significantly greater than that obsd. in previously known .sigma.-bonded diorgano Group 14 derivs. The compds. 4 and 5 are the 1st fully structurally characterized organometal **halide** derivs. of Ge or Sn in which the org. ligand is monodentate, purely .sigma.-bonded, and nonchelating.

L4 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1996:479406 CAPLUS

DN 125:221917

TI Isolation and Reduction of Sterically Encumbered Arylboron Dihalides: Novel Boranediyl Insertion into C-C .sigma.-Bonds

AU Grigsby, Warren J.; Power, Philip P.

CS Department of Chemistry, University of California, Davis, CA, 95616, USA

SO Journal of the American Chemical Society (1996), 118(34), 7981-7988

CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal
LA English
OS CASREACT 125:221917
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The **synthesis** and subsequent redn. of the arylboron dihalides 2,6-Mes2C6H3BX2 (X = Cl (1); Br (2)) and 2,6-Trip2C6H3BBBr2 (3) (Mes = 2,4,6-Me3C6H2- and Trip = 2,4,6-i-Pr3C6H2-) are described. Treatment of 2 with Li metal in Et2O gave the novel Li 9-borafluorenyl compds. 4 (shown as I) and 5 (shown as II) in which the boranediyl intermediate has inserted into an o-Me-ring C-C .sigma.-bond to form a borafluorenyl structure incorporating B in a delocalized five-membered ring. Boranediyl insertion into C-C .sigma.-bonds, as distinct from boranediyl induced rearrangements involving C:C cleavage in delocalized arom. substrates, is unknown. The main difference between the structures of these products is that 5 is dimerized as a consequence of the redn. in the no. of solvating ethers. Redn. of 2 with KC8 gave the 9-borafluorenyl ate compds. 6 and 7 (shown as III; L = THF, C6H6). These products also result from C-C bond insertion by B as seen in 4 and 5. However, the delocalization is not obsd. owing to the addn. of H (presumably from solvent) to the borons affording borate salts. Redn. of 3 with 3 equiv of KC8 furnishes the new diborate species 8 (shown as IV). This compd. features as unique B-B bonded dianionic structure with a long (1.83(2) .ANG.) B-B bond which arises from the assocn. of two borate radical anion fragments that have a 9-borafluorenyl structure similar to those described above. 2-8 Were characterized by 1H, 13C, 7Li, and 11B NMR spectroscopy and by x-ray crystallog.

L4 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1961:7917 CAPLUS

DN 55:7917

OREF 55:1521f-i,1522a-i,1523a-b

TI **Syntheses** with organolithium compounds obtained by substitution of a labile hydrogen atom

AU Ivanov, D.; Vasilev, G.; Panaiotov, I. M.; Borisov, G.; Marekov, N.

SO Godishnik Sofiiskiia Univ. Fiz.-Mat. Fak. (1959), Volume Date 1957-1958, 52(No. 3), 1-53

DT Journal

LA German

AB PhCHLiCO2Na (I), prepd. from an aromatic Li compd., and PhCH2CO2Na (II), reacted with Ph2CO (III) or CO2 to give Ph2C(OH)CHPhCO2H (IV) or PhCH(CO2H)2 (V), resp. I reacted also with PhCH2Bz (VI) (formed by the interaction of II and PhLi) to give PhCH2CPh(OH)CHPhCO2H (VII). Li (1.2 g.), 13.7 g. o-MeC6H4Br, 12.7 g. II, and 14.6 g. III in 100 ml. Et2O gave 64-7% IV, m. 187-8.degree.. The analogous use of .alpha.-ClOH7Br (VIII), 1,3,5-Me2BrC6H3, and 1,3,4,6-Me2Br2C6H2 afforded IV in 65-70, 72, and 33% yield, resp. Li (1.4 g.), 20.7 g. VIII, and 15.8 g. II in 120 ml. Et2O gave 42% impure V, m. 143-5.degree. (decompn.). Li (1.47 g.), 16.5 g. PhBr, and 16.6 g. II in 80 ml. Et2O gave 39-41% VII, m. 178.degree., and 21-3% VI, m. 56-7.5.degree. (EtOH). Alk. hydrolysis of VII afforded VI and PhCH2CO2H in quant. yield. PhCH2CR(OH)CHPhCO2H, and PhCH2COR were prepd. analogously from the appropriate aryl bromides (R, m.p., and % yield of acid, and m.p. and % yield of ketone listed): p-MeC6H4,

169-70.degree. (EtOH), 44-5, 107-9.degree., 25-33; m-MeC6H4, 149-51.degree., 40-3, 49-50.degree. (EtOH), 29-32, (semicarbazone m. 178-9.degree.); .alpha.-C10H7Br, 187.5-8.5.degree. (EtOH), 28 (crude) (use of Mg instead of Li gave 53% crude yield), -, -; p-MeOC6H4, 176-7.degree. (EtOH), 38 (crude), -, -; p-Me2NC6H4, -, -, 161-3.degree. (EtOH), 55 (oxime m. 140-2.degree.). o-MeC6H4Br and VIII did not yield any acid. PhLi (from 1.57 g. PhBr and 0.17 g. Li in 40 ml. Et2O) and 2.08 g. .alpha.-C10H7CH2CO2Na (IX) treated after 5 hrs. with solid CO2 gave 38% crude .alpha.-C10H7CH(CO2H)2 (X), m. 154.degree. (C6H6), and 12% .alpha.-C10H7CH2Bz, m. 105-6.degree. (EtOH); oxime m. 138-9.degree.. The analogous reactions of IX with Li derivs. of o-, m-, and p-MeC6H4Br, VIII, and p-Me2NC6H4Br yielded 42.2, 35, 19.5, 37.4, and 29.1% X, resp. The same amts. of PhBr, Li, and IX gave with 1.83 g. III after 3 hrs. 57% Ph2C(OH)CH(C10H7.alpha.)CO2H (XI), m. 159-60.degree. (EtOH). Similar reactions with PhAc, camphor, or VI failed to yield .beta.-hydroxy acids. PhLi (from 1.57 g. PhBr) and 2.08 g. .beta.-C10H7CH2CO2Na (XII) in Et2O treated with CO2 afforded 17.7-20% .beta.-C10H7CH(CO2H)2 (XIII), m. 155-6.degree. (decompn.) and 27.4% .beta.-C10H7CH2Bz, m. 122-3.degree. (EtOH). Similarly, XI and Li derivs. of o-, m-, and p-MeC6H4Br, VIII, and p-Me2NC6H4Br gave XIII in 48, 19.6, 21.7, 26.1, and 18.5% yield, resp. XII, III, and Li derivs. of PhBr, o-, and m-MeC6H4Br yielded 20.5, 18.3, and 17.2% Ph2C(OH)CH(C10H7.beta.)CO2H, m. 189-90.degree. (EtOH). PhBz and camphor, used instead of III, failed to give the analogous reaction. Aliphatic derivs. of Li behaved as the aromatic ones. Li (0.8 g.), 7.9 g. II, 9.1 g. III, and 0.05 mole alkyl **halide** in Et2O or a mixed solvent (ether-pentane, dioxane-pentane) gave IV; the alkyl **halide** used and % yield were the following: MeI, 3.3; EtBr, 18-21; PrCl, 42-8; iso-Pr, 23-5; BuCl, 46-52; EtCHClMe, 18; Me3CCl, 12-14; Me2CHCH2CH2Br, 35; cyclohexyl bromide, 20. Li (0.8 g.), 7.9 g. II, and 0.05 mole BuCl or PrCl in Et2O yielded 30 and 25% V, resp. Li (0.8 g.), 4.7 g. BuCl, and 7.9 g. II in 80 ml. Et2O refluxed then decompd. with ice-HCl gave 34% PhCH2CBu(OH)CHPhCO2H, m. 145-6.degree. (PhMe); alk. cleavage of this hydroxy acid gave PhCH2CO2H and PhCH2COBu; semicarbazone, needles, m. 114-15.degree. (aq. EtOH). A 50% excess of the Li deriv. at -10.degree. raised the yield to 55%. The following PhCH2CR(OH)CHPhCO2H were prepd. similarly (R **halide** used, m.p., yield of the hydroxy acid, and m.p. of the semicarbazone of PhCH2COR listed): PrCl, 160-1.degree. (aq. EtOH), 48, 121-2.degree. (MeOH); iso-Pr, 135-7.degree. (aq. EtOH), 28-31, 138-9.degree. (EtOH); EtCHClMe, 139-40.degree. (aq. EtOH), 28-39, 110-12.degree.. BuLi reacted with IX or XII in dioxane but failed to react in pentane or Et2O without the addn. of this solvent. Li (0.182 g.), 1.36 g. BuCl, and 20.8 g. IX in 15 ml. pentane and 10 ml. dioxane dild. with 50 ml. Et2O then treated with solid CO2 gave 6.5% X. The same amts. of Li, BuCl, IX, and solvents (without Et2O) treated with III gave 40.7% XI. Similarly, PrCl gave 45.3% XI iso-PrCl 15.6%, Me2CHCH2CH2Br 10%; MeI failed to react. Likewise, XIV was prepd. from XII (alkyl **halide** used and % yield as follows): PrCl, 37; iso-PrCl, 8.3; BuCl, 31.5; Me2CHCH2CH2Br, 27.6. MeLi (from 0.8 g. Li and 7.1 g. MeI) and 5.85 g. PhCH2CN (XV) in 90 ml. Et2O treated with solid CO2 gave 38-40% PhCH(CN)CO2H, m. 92.degree. (benzene). Similar yields were obtained with Li compds. prepd. from PrCl, BuCl, PhBr, o-MeC6H4Br, and VIII. Li (0.7 g.), 5.64 g. BuCl, 4.63 g. XV, and 9.1 g. III in 110 ml. Et2O gave 30% Ph2C:CPHCN, m. 165-6.degree. (EtOH). The analogous reactions of org. Li or Mg derivs. with .alpha.-C10H7CH2CN (XVI) gave .alpha.-C10H7CH(CN)CO2H, m. 130.5-1.0.degree. (benzene) (org. **halide** used, % yield of Li derivs. and Mg derivs. given): PrCl, 37.9, 17.5; iso-PrCl, -, 33.2; BuCl, 54.5, 25.7; PhBr, 50.0, 30.6; o-MeC6H4Br, 23.7, 29.4; VIII, 41.2, 35.6. Li (0.14 g.), 1.57 g. PhBr, 1.67 g. XVI, and 1.82 g. III in 40 ml. Et2O

gave 21.2% $\text{Ph}_2\text{C}(\text{OH})\text{CH}(\text{C}_{10}\text{H}_7.\alpha.)\text{CN}$, m. 179-80.degree.. Li (0.4 g.), 2.4 g. BuCl , and 3.95 g. II in 120 ml. Et_2O refluxed 4 hrs., 5.2 g. PhCH:CHBz added, and the mixt. refluxed 6 hrs. gave 38% crude $\text{BzCH}_2\text{CHPhCHPhCO}_2\text{H}$, m. 257-9.degree. (EtOH), and 22% low melting isomer, m. 186-7.degree. (benzene). When this reaction was carried out with iso- PrCl and Mg , the yields were 42 and 26% for the former and latter isomers, resp. BuLi , II (as above), and 5.8 g. $p\text{-MeOC}_6\text{H}_4\text{CH:CHBz}$ gave 29% $\text{BzCH}_2(p\text{-MeOC}_6\text{H}_4)\text{CHCHPhCO}_2\text{H}$, m. 225-6.5.degree. (EtOH), and 16% isomer, m. 205.5-6.5.degree. (benzene). Li (0.35 g.), 5.13 g. $o\text{-MeC}_6\text{H}_4\text{Br}$, and 3.95 g. II gave (a) with 6.1 g. $p\text{-ClC}_6\text{H}_4\text{CH:CHBz}$ 51% $\text{BzCH}_2(p\text{-ClC}_6\text{H}_4)\text{CHCHPhCO}_2\text{H}$, m. 242-3.degree. (AcOH), and 28% isomer, m. 210-11.degree. (benzene), and (b) with 5.85 g. $(\text{PhCH:CH})_2\text{CO}$ 45% $\text{PhCH:CHCOCH}_2\text{CHPhCHPhCO}_2\text{H}$, m. 254-5.degree. (EtOH), and 22% isomer, m. 214-15.degree. (benzene- EtOH). $o\text{-MeC}_6\text{H}_4\text{Li}$, II, and RCH_2Cl (20% excess) gave $\text{PhCH}_2\text{CHRCO}_2\text{H}$ (R, m.p., and % yield listed): Ph , 88-9.degree. (CHCl_3), 75-7 (when iso- PrMgCl was used yield was 30%); $o\text{-ClC}_6\text{H}_4$, 121-2.degree. (Et_2O -petr. ether), 71-4; $p\text{-ClC}_6\text{H}_4$, 140-150.5.degree. (sic) (aq. EtOH), 70-2; $p\text{-NCC}_6\text{H}_4$, 128-9.degree. (water), 80-5. Li, VIII, II, and RN:CHPh refluxed 6 hrs. in Et_2O gave $\text{RNHCHPhCHPhCO}_2\text{H}$ (R, m.p., and % yield given): Ph (XVII), 157-8.degree. (aq. EtOH), 74; $p\text{-MeC}_6\text{H}_4$, 178-80.degree. (aq. EtOH), 60; .beta.- C_{10}H_7 , 156-7.degree. (EtOH) (HCl salt m. 188-90.degree.), 70; $p\text{-MeOC}_6\text{H}_4$, 141-3.degree. (aq. EtOH), 78. XVII (1 g.) refluxed 6 hrs. with 30 ml. Ac_2O gave 0.6 g. $\text{PhCH:CPhCO}_2\text{H}$, m. 171-2.degree. (aq. EtOH). Li (0.14 g.), 2.07 g. VIII, and 1.58 g. II in 35 ml. Et_2O treated with 0.7 g. iodine then decompd. after 1 hr. gave 52.6% $(\text{CHPhCO}_2\text{H})_2$ (XVIII). The use of Mg instead of Li gave 17% XVIII. Similarly, 0.01 mole each Li, PhBr , IX, and iodine gave 30.3% (10.3% with Mg) (.alpha.- $\text{C}_{10}\text{H}_7\text{CHCO}_2\text{H})_2$ (XIX). Under the same conditions, XII yielded 27.5% (11.9% with Mg) .beta.-naphthyl isomer, m. 238.degree. (pyridine). Li and Mg derivs., prepd. from 0.01 mole II or IX (prepd. through VIII, or PhBr), were treated with N-bromosuccinimide (XX) in refluxing Et_2O . At the molar ratio of XX-II of 1.5:1, both meso- and dl-XVIII were obtained in 14.8, and 7.3% yield, resp. IX gave 11.5% meso- and 5.1% dl-XIX. Mg gave poorer results.

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1958:29887 CAPLUS

DN 52:29887

OREF 52:5352i,5353a-b

TI **Syntheses** with organolithium compounds by substitution of labile hydrogen. IX. **Syntheses** with .alpha.-lithiophenylacetonitrile

AU Ivanov, D.; Vasilev, G.

CS Univ. Sofia

SO Doklady Bolgarskoi Akademii Nauk (1957), 10(No. 1), 53-6

CODEN: DBANAD; ISSN: 0366-8681

DT Journal

LA German

AB cf. C.A. 52, 1974d. RLi (R = Me, Pr, Bu, Ph, .omicron.- MeC_6H_4 , .alpha.- C_{10}H_7) with PhCH_2CN gave PhCHLiCN , confirmed by reaction with solid CO_2 to give $\text{PhCH}(\text{CN})\text{CO}_2\text{H}$ and with Ph_2CO to give $\text{Ph}_2\text{C:CPhCN}$. The alkyl or aryl halide, RX, (0.05 mole in 30 cc. Et_2O) was added during 40-50 min. to 0.80 g. finely divided Li and 20-30 cc. Et_2O under N; after 40-50 min., 0.05 mole PhCH_2CN in 40 cc. Et_2O was added dropwise in 15 min., the mixt. stirred 3 hrs. at room temp., the yellow soln. poured on solid CO_2 , acidified with dil. HCl , extd. with dil. alkali, again acidified and extd. with Et_2O , and the residue crystd. from C_6H_6 giving 38-47% $\text{PhCH}(\text{CN})\text{CO}_2\text{H}$, m. 91-2.degree.. Because of the much less acidic character of CH_2 in $\text{PhCH}_2\text{CO}_2\text{Na}$ the yield of $\text{PhCHLiCO}_2\text{Na}$ in a similar

reaction was only 3.3%. Excess BuCl with Li, PhCH₂CN, and Ph₂CO in Et₂O gave 30% Ph₂C:CPhCN, m. 163-4.degree., formed by dehydration of Ph₂C(OH)CHPhCN.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

60.04

60.25

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

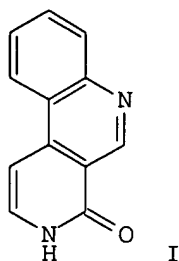
CA SUBSCRIBER PRICE

-3.91

-3.91

STN INTERNATIONAL LOGOFF AT 11:46:29 ON 21 NOV 2003

L17 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1994:134231 CAPLUS
 DN 120:134231
 TI First metalation of aryl iodides: directed ortho-lithiation of
 iodopyridines, halogen-dance, and application to **synthesis**
 AU Rocca, P.; Cochenec, C.; Marsais, F.; Thomas-dit-Dumont, L.; Mallet, M.;
 Godard, A.; Queguiner, G.
 CS Lab. Chim. Org. Heterocycl., Inst. Chim. Org. Fine, Mont-Saint-Aignan,
 76131, Fr.
 SO Journal of Organic Chemistry (1993), 58(27), 7832-8
 CODEN: JOCEAH; ISSN: 0022-3263
 DT Journal
 LA English
 OS CASREACT 120:134231
 GI



AB Metalation of iodopyridines was successfully achieved by LDA at low temp. In many cases, lithiation is ortho directed by the iodo group which subsequently ortho-migrates very fast to give stabilized iodolithiopyridines. This procedure was applied to 2-fluoro- and 2-chloro-3-iodopyridines, 3-fluoro-4-iodopyridine, and 2-chloro-3-fluoro-4-iodopyridine. The resulting lithio intermediates were obtained in high yields before being reacted with electrophiles leading to various polysubstituted pyridines. Some of these iodopyridines were used as key mols. for the prepn. of fused polyarom. alkaloids. Thus, perolidine (I), .delta.-carboline, and 2,10-diazaphenanthrenes were readily prepd. in few steps taking advantage of the iodo reactivity for heteroring cross-coupling. Coupling of [2-(pivaloylamino)**phenyl**]boronic acid with 2-fluoro-4-iodo-3-pyridinecarboxaldehyde gave I.

=> s synthesis and phenyl boronic acid and production

L18 0 SYNTHESIS AND PHENYL BORONIC ACID AND PRODUCTION

=> s synthesis and phenyl boronic acid

L19 69 SYNTHESIS AND PHENYL BORONIC ACID

=> s l19 and one pot

L20 3 L19 AND ONE POT

=> d l20 fbib hitstr abs rtotat

'RTOTAL' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

Welcome to STN International! Enter x:x

LOGINID:ssspta1611sxp

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 09	CA/CAPlus records now contain indexing from 1907 to the present
NEWS	4	AUG 05	New pricing for EUROPATFULL and PCTFULL effective August 1, 2003
NEWS	5	AUG 13	Field Availability (/FA) field enhanced in BEILSTEIN
NEWS	6	AUG 18	Data available for download as a PDF in RDISCLOSURE
NEWS	7	AUG 18	Simultaneous left and right truncation added to PASCAL
NEWS	8	AUG 18	FROSTI and KOSMET enhanced with Simultaneous Left and Right Truncation
NEWS	9	AUG 18	Simultaneous left and right truncation added to ANABSTR
NEWS	10	SEP 22	DIPPR file reloaded
NEWS	11	SEP 25	INPADOC: Legal Status data to be reloaded
NEWS	12	SEP 29	DISSABS now available on STN
NEWS	13	OCT 10	PCTFULL: Two new display fields added
NEWS	14	OCT 21	BIOSIS file reloaded and enhanced
NEWS	15	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS EXPRESS		NOVEMBER 14	CURRENT WINDOWS VERSION IS V6.01c, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
NEWS INTER			General Internet Information
NEWS LOGIN			Welcome Banner and News Items
NEWS PHONE			Direct Dial and Telecommunication Network Access to STN
NEWS WWW			CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:51:14 ON 21 NOV 2003

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

Patel

<11/20/2003>

FILE 'REGISTRY' ENTERED AT 10:51:20 ON 21 NOV 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 20 NOV 2003 HIGHEST RN 619253-33-7
DICTIONARY FILE UPDATES: 20 NOV 2003 HIGHEST RN 619253-33-7

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

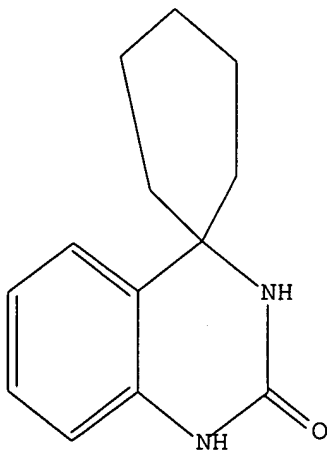
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP
PROPERTIES for more information. See STN Note 27, Searching Properties
in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=>
Uploading 10101996.1

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> file caplus
COST IN U.S. DOLLARS
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
0.40	0.61

Patel

<11/20/2003>

FILE 'CAPLUS' ENTERED AT 10:51:52 ON 21 NOV 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 21 Nov 2003 VOL 139 ISS 22
FILE LAST UPDATED: 20 Nov 2003 (20031120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s lithium and aryl halides
L2 172 LITHIUM AND ARYL HALIDES

=> s lithium and fluoro phenyl
L3 12 LITHIUM AND FLUORO PHENYL

=> s phenyl boronic acid and phenyl borinic acid
L4 0 PHENYL BORONIC ACID AND PHENYL BORINIS ACID

=> s pheny boronic acid
L5 0 PHENY BORONIC ACID

=> s phenyl boronic acid
L6 233 PHENYL BORONIC ACID

=> s phenyl borinic acid
L7 3 PHENYL BORINIC ACID

=> s l6 and l7
L8 0 L6 AND L7

=> s l3 and l6
L9 0 L3 AND L6

=> s l3 and l2
L10 0 L3 AND L2

=> s l2 and phenyl boronic acid
L11 1 L2 AND PHENYL BORONIC ACID

=> s l2 and phenyl borinic acid
L12 0 L2 AND PHENYL BORINIC ACID

=> s l2 and l6

L13 1 L2 AND L6

=> s l3 and l6

L14 0 L3 AND L6

=> s l2 and l6

L15 1 L2 AND L6

=> s l15 fbib hitstr abs total

MISSING OPERATOR L15 FBIB

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> d l15 fbib hitstr abs total

L15 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2000:261550 CAPLUS

DN 133:30370

TI Biaryls via Suzuki cross-couplings catalyzed by nickel on charcoal

AU Lipshutz, Bruce H.; Sclafani, Joseph A.; Blomgren, Peter A.

CS Department of Chemistry & Biochemistry, University of California, Santa Barbara, CA, 93106-9510, USA

SO Tetrahedron (2000), 56(15), 2139-2144

CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 133:30370

AB Using the heterogeneous catalyst Ni/C, biaryl bonds can be made between functionalized aryl chlorides and boronic acids in good isolated yields. A std. set of conditions was developed which applies to a variety of reaction partners. For example, the coupling reaction of 1-chloro-4-methoxybenzene with phenylboronic acid in the presence of nickel/charcoal and **lithium** bromide gave 4-methoxy-[1,1'-biphenyl]. Similarly, coupling of (4-methoxyphenyl)diphenylphosphine with phenylboronic acid also gave 4-methoxy-[1,1'-biphenyl] in good yield.

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> s phenyl boronic acid and synthesis

L16 69 PHENYL BORONIC ACID AND SYNTHESIS

=> s l16 and lithium

L17 2 L16 AND LITHIUM

=> d l17 fbib hitstr abstotal

'ABSTOTAL' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB

ALL ----- BIB, AB, IND, RE

APPS ----- AI, PRAI

BIB ----- AN, plus Bibliographic Data and PI table (default)

CAN ----- List of CA abstract numbers without answer numbers

CBIB ----- AN, plus Compressed Bibliographic Data

DALL ----- ALL, delimited (end of each field identified)

DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, IPC, and NCL

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

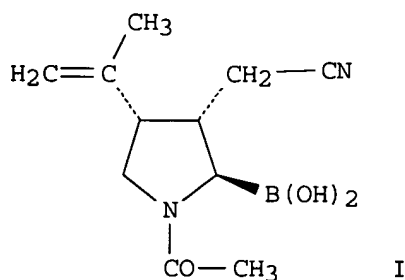
All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):BIB

L17 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:557500 CAPLUS
DN 129:245183
TI Asymmetric **synthesis** of 1-acyl-3,4-disubstituted
pyrrolidine-2-boronic acid derivatives
AU Matteson, Donald S.; Lu, Jianhui

CS Department of Chemistry, Washington State University, Pullman, WA,
99164-4630, USA
SO Tetrahedron: Asymmetry (1998), 9(14), 2423-2436
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 129:245183
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 117 fbib hitstr abs total

L17 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:557500 CAPLUS
DN 129:245183
TI Asymmetric **synthesis** of 1-acyl-3,4-disubstituted
pyrrolidine-2-boronic acid derivatives
AU Matteson, Donald S.; Lu, Jianhui
CS Department of Chemistry, Washington State University, Pullman, WA,
99164-4630, USA
SO Tetrahedron: Asymmetry (1998), 9(14), 2423-2436
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 129:245183
GI



AB An analog of N-acetylkainic acid having a cyano group and a boronic acid group in place of the two carboxyl groups, e.g., I, was synthesized with high stereocontrol via chain extensions of pinanediol [(trityloxy)methyl]boronate with (dihalomethyl)**lithium** followed by appropriate nucleophilic substitution of the resulting chloro or bromo boronic ester. Substituents were introduced in the order isopropenyl, cyanomethyl, and bis(trimethylsilyl)amino. The last of these was converted to acetamido, the hydroxyl function was unmasked and mesylated, and the pyrrolidine ring was closed. Attempts to carry out further chain extension on the boronic ester resulted in low yields, evidently the highly polar amido substituent interferes with the (dichloromethyl) **lithium** insertion process.
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

The following are valid formats:

```

ABS ----- GI and AB
ALL ----- BIB, AB, IND, RE
APPS ----- AI, PRAI
BIB ----- AN, plus Bibliographic Data and PI table (default)
CAN ----- List of CA abstract numbers without answer numbers
CBIB ----- AN, plus Compressed Bibliographic Data
DALL ----- ALL, delimited (end of each field identified)
DMAX ----- MAX, delimited for post-processing
FAM ----- AN, PI and PRAI in table, plus Patent Family data
FBIB ----- AN, BIB, plus Patent FAM
IND ----- Indexing data
IPC ----- International Patent Classifications
MAX ----- ALL, plus Patent FAM, RE
PATS ----- PI, SO
SAM ----- CC, SX, TI, ST, IT
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
          SCAN must be entered on the same line as the DISPLAY,
          e.g., D SCAN or DISPLAY SCAN)
STD ----- BIB, IPC, and NCL

IABS ----- ABS, indented with text labels
IALL ----- ALL, indented with text labels
IBIB ----- BIB, indented with text labels
IMAX ----- MAX, indented with text labels
ISTD ----- STD, indented with text labels

OBIB ----- AN, plus Bibliographic Data (original)
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations
SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms
HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
          containing hit terms
HITRN ----- HIT RN and its text modification
HITSTR ----- HIT RN, its text modification, its CA index name, and
          its structure diagram
HITSEQ ----- HIT RN, its text modification, its CA index name, its
          structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
          its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
          structure diagram, plus NTE and SEQ fields
KWIC ----- Hit term plus 20 words on either side
OCC ----- Number of occurrence of hit term and field in which it occurs

```

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC

to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):BIB

L20 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:384384 CAPLUS
DN 139:230701
TI Pyridazines. Part 34: Retro-ene-assisted palladium-catalyzed
synthesis of 4,5-disubstituted-3(2H)-pyridazinones
AU Sotelo, Eddy; Coelho, Alberto; Ravina, Enrique
CS Facultad de Farmacia, Departamento de Quimica Organica, Laboratorio de
Quimica Farmaceutica, Universidad de Santiago de Compostela, Santiago de
Compostela, 15782, Spain
SO Tetrahedron Letters (2003), 44(24), 4459-4462
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d l20 fbib hitstr abs total

L20 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:384384 CAPLUS
DN 139:230701
TI Pyridazines. Part 34: Retro-ene-assisted palladium-catalyzed
synthesis of 4,5-disubstituted-3(2H)-pyridazinones
AU Sotelo, Eddy; Coelho, Alberto; Ravina, Enrique
CS Facultad de Farmacia, Departamento de Quimica Organica, Laboratorio de
Quimica Farmaceutica, Universidad de Santiago de Compostela, Santiago de
Compostela, 15782, Spain
SO Tetrahedron Letters (2003), 44(24), 4459-4462
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
AB The efficient **one-pot** bis-functionalization of the
4,5-positions of the 3-pyridazinone ring has been performed using Suzuki,
Sonogashira h Sonogashira and Stille cross-coupling reactions assisted by
a retro-ene fragmentation. This route allows access in a shorter
synthetic sequence to several pharmacol. useful 3(2H)-pyridazinones. The
treatment of 4,5-dibromo-2-(hydroxymethyl)-3(2H)-pyridazinone or
4,5-dichloro-2-(hydroxymethyl)-3(2H)-pyridazinone with arylboronic acid
derivs. gave 4,5-diaryl-3(2H)-pyridazinone derivs. whereby the
hydroxymethyl group was lost as formaldehyde via said retro-ene
fragmentation.
RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:960932 CAPLUS
DN 138:137250
TI Pyridazines. Part 30: palladium-catalysed **synthesis** of
5-substituted 6-phenyl-3(2H)-pyridazinones assisted by a retro-ene
transformation
AU Coelho, Alberto; Ravina, Enrique; Sotelo, Eddy
CS Laboratorio de Quimica Farmaceutica, Departamento de Quimica Organica,

Facultad de Farmacia, Universidad de Santiago de Compostela, Santiago de Compostela, 15782, Spain

SO Synlett (2002), (12), 2062-2064

CODEN: SYNLES; ISSN: 0936-5214

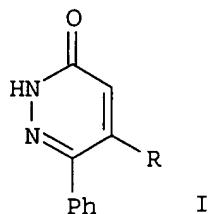
PB Georg Thieme Verlag

DT Journal

LA English

OS CASREACT 138:137250

GI



AB The efficient **one-pot** functionalization, through palladium-catalyzed ($\text{Pd}(\text{PPh}_3)_4$ and $\text{PdCl}_2(\text{PPh}_3)_2$) Suzuki, Sonogashira and Stille coupling reactions, of position 5 of the 6-phenyl-3(2H)-pyridazinone system I ($\text{R} = \text{Ph}$, 4-MeC₆H₄, 4-ClC₆H₄, 4-OHCC₆H₄, C.tplbond.C-TMS, C.tplbond.C-CH₂OH, C.tplbond.C-CH(OEt)₂, CH=CH₂) has been performed using a retro-ene-assisted fragmentation. This route allows access through a short synthetic sequence to several pharmacol. useful 3(2H)-pyridazinones.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L20 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:925161 CAPLUS

DN 138:338108

TI **Synthesis** of some diazino-fused tricyclic systems via Suzuki cross-coupling and regioselective nitrene insertion reactions

AU Tapolcsanyi, Pal; Krajsovsky, Gabor; Ando, Romeo; Lipcsey, Peter; Horvath, Gyula; Matyus, Peter; Riedl, Zsuzsanna; Hajos, Gyorgy; Maes, Bert U. W.; Lemiere, Guy L. F.

CS Department of Organic Chemistry, Semmelweis University, Budapest, 1092, Hung.

SO Tetrahedron (2002), 58(51), 10137-10143

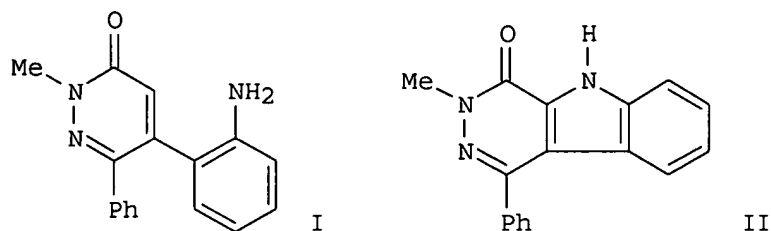
CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

GI



AB Suzuki coupling of 5-chloro-2-methyl-6-phenylpyridazin-3(2H)-one, 6-chloro-1,3-dimethyluracil and 2-chloropyrazine with protected aminoaryl boronic acids resulted in the corresponding (pivaloylamino)phenyl diazines which were transformed to diazino-fused indole and cinnoline derivs. Suzuki coupling of 5-amino-6-chloro-1,3-dimethyluracil with 2-formylphenyl boronic acid afforded a novel pyrimidoisoquinoline ring system in a **one-pot** reaction. For example, Suzuki coupling of 5-chloro-2-methyl-6-phenyl-3(2H)-pyridazinone with [2-[(2,2-dimethyl-1-oxopropyl)amino]phenyl]boronic acid gave 2-methyl-6-phenyl-5-[2-(pivaloylamino)-3(2H)-pyridazinone which was deprotected to give 5-(2-aminophenyl)-2-methyl-6-phenyl-3(2H)-Pyridazinone (I). Diazotization and sequential azidization of I gave 5-(2-azidophenyl)-2-methyl-6-phenyl-3(2H)-pyridazinone which was cyclized to give 3,5-dihydro-3-methyl-1-phenyl-4H-pyridazino[4,5-b]indol-4-one (II).

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 10:51:14 ON 21 NOV 2003)

FILE 'REGISTRY' ENTERED AT 10:51:20 ON 21 NOV 2003

L1 STRUCTURE UPLOADED

FILE 'CAPLUS' ENTERED AT 10:51:52 ON 21 NOV 2003

L2 172 S LITHIUM AND ARYL HALIDES
L3 12 S LITHIUM AND FLUORO PHENYL
L4 0 S PHENYL BORONIC ACID AND PHENYL BORINIS ACID
L5 0 S PHENY BORONIC ACID
L6 233 S PHENYL BORONIC ACID
L7 3 S PHENYL BORINIC ACID
L8 0 S L6 AND L7
L9 0 S L3 AND L6
L10 0 S L3 AND L2
L11 1 S L2 AND PHENYL BORONIC ACID
L12 0 S L2 AND PHENYL BORINIC ACID
L13 1 S L2 AND L6
L14 0 S L3 AND L6
L15 1 S L2 AND L6
L16 69 S PHENYL BORONIC ACID AND SYNTHESIS
L17 2 S L16 AND LITHIUM
L18 0 S SYNTHESIS AND PHENYL BORONIC ACID AND PRODUCTION
L19 69 S SYNTHESIS AND PHENYL BORONIC ACID
L20 3 S L19 AND ONE POT

```
=> s lithium and phenyl halide
L21      12 LITHIUM AND PHENYL HALIDE

=> s lithium and aryl halides
L22      172 LITHIUM AND ARYL HALIDES

=> s lithium aryl halides
L23      0 LITHIUM ARYL HALIDES

=> s aryl lithium halise and boronic acids
L24      0 ARYL LITHIUM HALISE AND BORONIC ACIDS

=> s aryl lithium halides and boronic acids
L25      0 ARYL LITHIUM HALIDES AND BORONIC ACIDS

=> s l21 and l22
L26      4 L21 AND L22

=> s lithium and grignard reagent
L27      1118 LITHIUM AND GRIGNARD REAGENT

=> s l27 and phenyl boronic acid
L28      0 L27 AND PHENYL BORONIC ACID

=> s l27 and phenyl borinic acid
L29      0 L27 AND PHENYL BORINIC ACID

=> s phenyl boronic acid ans synthesis
L30      0 PHENYL BORONIC ACID ANS SYNTHESIS

=> s phenyl boronic acid and synthesis
L31      69 PHENYL BORONIC ACID AND SYNTHESIS

=> s l31 and l27
L32      0 L31 AND L27

=> s l31 and litium
L33      0 L31 AND LITIUM

=> s l31 and phenyl lithium fluoride
L34      0 L31 AND PHENYL LITHIUM FLUORIDE

=> s lithium and fluorophenyl
L35      317 LITHIUM AND FLUOROPHENYL

=> s l35 and synthesis
L36      90 L35 AND SYNTHESIS

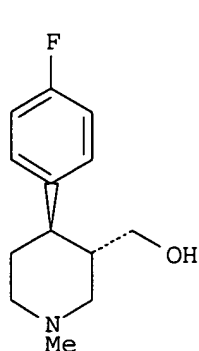
=> s l36 and reagent
L37      16 L36 AND REAGENT

=> s l37 fbib hitstr abs total
MISSING OPERATOR L37 FBIB
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

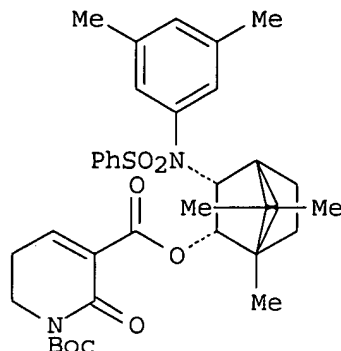
=> d l37 fbib hitstr abs total
```

L37 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:509067 CAPLUS
DN 139:216147
TI The **Synthesis** of N-Aryl-5(S)-aminomethyl-2-oxazolidinone
Antibacterials and Derivatives in One Step from Aryl Carbamates
AU Perrault, William R.; Pearlman, Bruce A.; Godrej, Delara B.; Jeganathan,
Azhwarsamy; Yamagata, Koji; Chen, Jiong J.; Lu, Cuong V.; Herrinton, Paul
M.; Gadwood, Robert C.; Chan, Lai; Lyster, Mark A.; Maloney, Mark T.;
Moeslein, Jeffery A.; Greene, Meredith L.; Barbachyn, Michael R.
CS Early Chemical Process Research and Development, Chemical Process Research
and Development, and Medicinal Chemistry Research, Pharmacia Corporation,
Kalamazoo, MI, 49001, USA
SO Organic Process Research & Development (2003), 7(4), 533-546
CODEN: OPRDFK; ISSN: 1083-6160
PB American Chemical Society
DT Journal
LA English
AB Economical methods for the large-scale prepn. of N-[(2S)-2-(acetyloxy)-3-
chloropropyl]acetamide and tert-Bu [(2S)-3-chloro-2-
hydroxypropyl]carbamate from com. available (S)-epichlorohydrin via the
common intermediate (2S)-1-amino-3-chloro-2-propanol hydrochloride were
developed. General methods for coupling these **reagents** with
N-aryl carbamates to give N-aryl-5(S)-aminomethyl-2-oxazolidinone derivs.
in one step were developed. These **reagents** and procedures have
proven widely applicable in the prepn. of a diverse array of oxazolidinone
analogs in both process and medicinal chem. research.
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:149737 CAPLUS
DN 139:85211
TI Diastereoselective conjugate addition of organocuprates to chiral racemic
olefinic amido esters. Formal total **synthesis** of paroxetine
AU Cossy, Janine; Mirguet, Olivier; Pardo, Domingo Gomez; Desmurs, Jean-Roger
CS Laboratoire de Chimie Organique, ESPCI, Paris, 75231, Fr.
SO New Journal of Chemistry (2003), 27(3), 475-482
CODEN: NJCHE5; ISSN: 1144-0546
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 139:85211
GI



I



II

AB Racemic fluorophenylpiperidinemethanol I is prepd. diastereoselectively using the addn. of a fluorophenylcuprate to dihydropyridinonecarboxylate II contg. an (arylsulfonylamino)borneoxy auxiliary as the key step. Boc protection of .delta.-valerolactam, lithiation and methoxycarbonylation with Me chlorocarbonate, ester exchange with a racemic (arylsulfonylamino)borneol auxiliary, .alpha.-phenylselenation, and peroxide-mediated oxidn. followed by thermal elimination of the phenylselenoxide group yield II in five steps. Addn. of a cuprate **reagent** prepd. by lithiation of 4-fluorophenyl bromide followed by exchange with copper (I) iodide to II yields a racemic oxopiperidinedicarboxylate in 80% yield. Redn. of the oxopiperidinedicarboxylate with **lithium** aluminum hydride yields I; since previous **syntheses** of paroxetine also use I as an intermediate, the prepn. of I constitutes a formal **synthesis** of racemic paroxetine. The use of a nonracemic (arylsulfonylamino)borneol auxiliary allows access to nonracemic (-)-paroxetine (no data).

RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2003:131813 CAPLUS

DN 138:172798

TI **Synthesis** of trialkyl- and triaryl-substituted boranes, boronic acids, and tetraalkylborates in flow-through reactors

IN Koch, Manfred; Wehle, Detlef; Scherer, Stefan; Forstinger, Klaus; Meudt, Andreas

PA Clariant G.m.b.H., Germany

SO Ger. Offen., 6 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10139664	A1	20030220	DE 2001-10139664	20010811
	EP 1285925	A1	20030226	EP 2002-16150	20020720
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	US 2003069420	A1	20030410	DE 2001-10139664A	20010811
				US 2002-210435	20020801
				DE 2001-10139664A	20010811
	JP 2003113185	A2	20030418	JP 2002-234590	20020812
				DE 2001-10139664A	20010811

OS MARPAT 138:172798
 AB Manuf. of arylboron and alkylboron compds., of general formulas R_nBX_{3-n} and R_4B-Li^+ , as well as $R_nB(OH)_{3-n}$ (prepd. by hydrolysis of R_nBX_{3-n}), are prepd. from the corresponding aryllithium and alkylolithium **reagents**, $R-Li$, and BX_3 , in which $X = F, Cl, Br, I, C1-5-alkoxy, N,N-di(C1-5-alkyl)amino, or (C1-5-alkyl)thio; n = 1, 2, or 3; and R = C1-6-alkyl, (RO-, RR'N-, Ph-, substituted Ph-, F-, and RS-), and (C1-6-alkyl)-substituted phenyl; and (C1-6-alkyl-, C1-6-alkoxy-, C1-5-thioalkyl-, silyl-, F-, Cl-, dialkylamino-, diarylamino-, and alkylarylamino)-substituted Ph, in addn. to heterocycloaryl substituents with one or two heteroatoms (e.g., N, O, or S). The compds. are synthesized in through-flow microreactors in flow channels of diam. 0.25 .mu. to 1.5 mm.$

L37 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:14172 CAPLUS

DN 136:200086

TI Convergent **Synthesis** of 6-Substituted Phenanthridines via Anionic Ring Closure

AU Lysen, Morten; Kristensen, Jesper L.; Vedso, Per; Begtrup, Mikael
 CS Department of Medicinal Chemistry, The Royal Danish School of Pharmacy, Copenhagen, DK-2100, Den.

SO Organic Letters (2002), 4(2), 257-259
 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

AB The addn. of organometallic derivs. to the cyano group of 2-(2-fluorophenyl)benzonitrile followed by intramol. nucleophilic substitution produces 6-substituted phenanthridines. Alkylolithiums, aryllithiums, and sterically nondemanding **lithium** amides reacted at -78 .degree.C to produce the 6-substituted phenanthridines in 82-98% yield upon warming to room temp. The addn. of the corresponding Grignard **reagents** requires an excess of the organometallic **reagent** and extended reaction times at elevated temp.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2001:730701 CAPLUS

DN 135:272866

TI **Synthesis** of $[R-(R^*, R^*)]-2-(4-fluorophenyl)-\beta,\delta-dihydroxy-5-(1-methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1H-pyrrole-1-heptanoic acid$ hemi calcium salt (atorvastatin)

IN Sambasivan, Ganesh; Sridharan, Madhavan; Padudevastana, Sathyashanker; Poornaprajna, Acharya; Mathew, Joy; Srinath, Sumithra; Nair, Satheesh

PA Biocon India Limited, India

SO PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001072706	A1	20011004	WO 2000-IN30	20000328
	W:	AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,			

IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
 MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
 SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZW, AM,
 AZ, BY, KG, KZ, MD, RU, TJ, TM
 RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
 DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
 CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

WO 2000-IN30

20000328

OS CASREACT 135:272866; MARPAT 135:272866

AB The present invention discusses a novel process for the **synthesis**
 of [R-(R*,R*)]-2-(4-**fluorophenyl**)-.beta.,.delta.-dihydroxy-5-(1-
 methylethyl)-3-phenyl-4-[(phenylamino)carbonyl]-1H-pyrrole-1-heptanoic
 acid hemi Ca salt by using 4-fluoro-.alpha.-[2-methyl-1-oxopropyl]-.gamma.-
 oxo-N-.beta.-diphenylbenzene butaneamide with Me (4R)-6-(2-aminoethyl)-2,2-
 dimethyl-1,3-dioxane-3-acetate. The compd. so prepd. is useful as
 inhibitors of the enzyme HMG-CoA reductase and are thus used as
 hypolipidemic and hypocholesterolemic agents.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 6 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2001:31487 CAPLUS

DN 134:102526

TI Process for the **synthesis** of citalopram

IN Bolzonella, Eva; Castellin, Andrea; Nicole, Andrea

PA Vis Farmaceutici S.p.A., Italy

SO PCT Int. Appl., 21 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001002383	A2	20010111	WO 2000-EP6426	20000706
	WO 2001002383	A3	20010503		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
				IT 1999-MI1486 A	19990706
	IT 99MI1486	A1	20010108	IT 1999-MI1486	19990706
	WO 2002004435	A1	20020117	WO 2001-DK481	20010706
	W:	AE, AG, AL, AM, AT, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
				WO 2000-EP6426 W	20000706

BR 2001006976	A	20020723	BR 2001-6976	20010706
			WO 2000-EP6426 A	20000706
			WO 2001-DK481 W	20010706
NO 2002001118	A	20020424	NO 2002-1118	20020306
			WO 2000-EP6426 A	20000706
			WO 2001-DK481 W	20010706
US 2002128497	A1	20020912	US 2002-96149	20020306
			WO 2000-EP6426 W	20000706
			WO 2001-DK481 A1	20010706

AB A new process is described for the **synthesis** of citalopram characterized by the conversion of 1-(4'-**fluorophenyl**)1-3-(dimethylaminopropyl)-5-halophthalane in the corresponding Grignard **reagent**; this intermediate product may be converted into citalopram via intermediate formation of an aldehyde and in the subsequent transformation of the functional group via oxime or hydrazone; or else be converted into citalopram via reaction with compds. contg. a cyano group bound to a leaving group. The process described makes it possible to obtain citalopram in high yields, and does not involve the use of drastic conditions of temp.

L37 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1999:585127 CAPLUS

DN 132:3536

TI **Synthesis** of enantiomerically pure .beta.- and .gamma.-amino acid derivatives using functionalized organozinc **reagents**

AU Dexter, Charles S.; Jackson, Richard F. W.; Elliott, Jason

CS Department of Chemistry, The University of Newcastle, Newcastle upon Tyne, NE1 7RU, UK

SO Journal of Organic Chemistry (1999), 64(20), 7579-7585

CODEN: JOCEAH; ISSN: 0022-3263

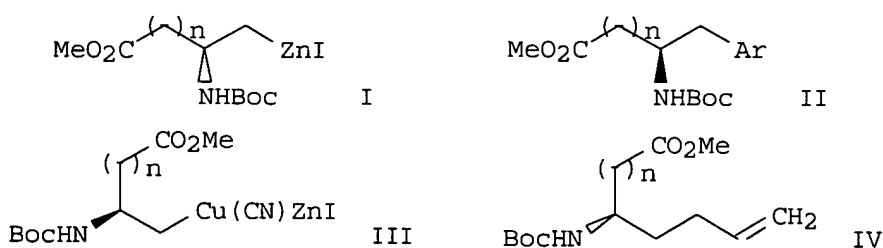
PB American Chemical Society

DT Journal

LA English

OS CASREACT 132:3536

GI

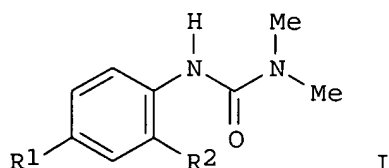


AB .beta.-Amido zinc **reagents** I (n = 1, 2) readily undergo .beta.-elimination when prepd. in THF, but when a polar aprotic solvent such as DMF is employed, .beta.-elimination is suppressed. Using DMF, reaction of I (n = 1) with ArI (Ar = Ph, C₆H₄Me-4, C₆H₄OMe-2, C₆H₄OMe-4, C₆H₄NH₂-2, C₆H₄F-2, C₆H₄NO₂-4, etc.) provides .beta.-homophenylalanine derivs. II (n = 1) in 20-89% yields; and analogous reactions of I (n = 2) with ArI give .gamma.-bishomophenylalanine derivs. II (n = 2) in 34-80% yields. The related zinc/copper **reagents** III (n = 1, 2) are also useful intermediates that undergo subsequent cross-coupling reactions with a wide range of electrophiles. For example, when the electrophile is

allyl chloride, products IV (n = 1, 2) are obtained in 82 and 87% yields, resp.

RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:497829 CAPLUS
DN 131:336798
TI Variation in site of lithiation with ring substituent of
N'-aryl-N,N-dimethylureas: application in **synthesis**
AU Smith, Keith; El-Hiti, Gamal A.; Shukla, Amba P.
CS Department of Chemistry, University of Wales Swansea, Swansea, SA2 8PP, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and
Bio-Organic Chemistry (1999), (16), 2305-2313
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
OS CASREACT 131:336798
GI



AB Lithiation of various N'-aryl-N,N-dimethylureas, I (R1 = Cl, F, CF₃, H, Me, MeO; R2 = H, Me) takes different courses depending on the substituent on the aryl ring. N'-(4-Chlorophenyl)-, N'-(4-fluorophenyl)- and N'-(4-trifluoromethylphenyl)-N,N-dimethylureas are doubly lithiated, on nitrogen and on the carbon at position 2, with n-butyllithium or tert-butyllithium at 0.degree.. The **lithium reagents** thus obtained react with a variety of electrophiles (iodomethane, D₂O, benzophenone, benzaldehyde, Ph isocyanate and Ph isothiocyanate) to give the corresponding 2-substituted derivs., in very good yields for the chloro and fluoro derivs. Reaction of the dilithio **reagent** of N'-(4-chlorophenyl)-N,N-dimethylurea with 2-chlorocyclohexanone gives an 82% isolated yield of 4a-hydroxy-N-(dimethylaminocarbonyl)-1,2,3,4,4a,9a-hexahydrocarbazole, which on treatment with trifluoroacetic acid affords N-(dimethylaminocarbonyl)-1,2,3,4-tetrahydrocarbazole in 97% yield. Double lithiation of N'-phenyl- and N'-(4-methylphenyl)-N,N-dimethylureas is achieved using tert-butyllithium at -20.degree., takes place on nitrogen and predominantly on one of the two Me groups of the urea. The **lithium reagents** so produced also react with a range of electrophiles to give the corresponding N-methyl-substituted compds. in very good yields. Lithiation of the N'-(4-methoxyphenyl)-analog with tert-butyllithium at 0.degree. or at -20.degree. takes place on nitrogen, and then partially on carbon at position 3 but primarily on a Me group of the urea, leading to a mixt. of ring substitution, Me substitution and di-substitution (in the ring and on the Me group) on reaction with representative electrophiles. However, disubstituted derivs. are obtained in very good yields when 3 molar equivalents of tert-butyllithium are used to form a trianion. Attempted lithiation of the N'-(4-nitrophenyl) analog

was not successful under various reaction conditions.

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1998:345620 CAPLUS
DN 129:161688
TI Enantioselective preparation of C2-symmetrical ferrocenyl ligands for asymmetric catalysis
AU Schwink, Lothar; Knochel, Paul
CS Fachbereich Chem., Philipps-Univ. Marburg, Marburg, D-35032, Germany
SO Chemistry--A European Journal (1998), 4(5), 950-968
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
OS CASREACT 129:161688
AB Corey-Bakshi-Shibata (CBS) redn. of the 1,1'-diacylmetallocenes of Fe and Ru (e.g. 1,1'-(ClCH₂CH₂CH₂C(O))₂ferrocene) provides the C2-sym. diols 4 (e.g. (R,R)-1,1'-(MeCH(OH))₂ferrocene) and 10, which proved to be useful starting materials for stereo-controlled ligand **synthesis**. Diols 4 and 10 can be easily converted to a wide range of diamines, diphosphines, and dithioacetates by nucleophilic substitution of the hydroxyl function with full retention of configuration. Also, the aminophosphines 30 (e.g. (.alpha.R,.alpha.'R)-2,2'-bis(.alpha.-(dimethylamino)(phenyl)methyl)-(S,S)-1,1'-bis(diphenylphosphino)ferrocene) and 31 (the Ru analog of the example for 30) become easily accessible. Compds. 30 and 31 were used as ligands complexed to Pd in enantioselective cross-coupling of racemic secondary Grignard **reagents** with vinyl bromides. A selectivity up to 93% ee could be reached for the 1st time in the prepn. of (S)-(E)-1,3-diphenyl-1-butene, which was transformed into the enantiomerically pure chiral building block (2R,4R)-2,4-diphenyl-3-pentanol with a pseudoasym. center in a straightforward, three-step **synthesis**.

RE.CNT 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:719685 CAPLUS
DN 128:13139
TI Method of preparing sulfonamides from sulfones
IN Huang, Horng-chih; Haring, Scott R.
PA G. D. Searle & Co., USA
SO U.S., 13 pp., Cont.-in-part of U.S. Ser. No. 275,183.
CODEN: USXXAM

DT Patent
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5684195	A	19971104	US 1995-455460	19950531
				US 1994-275183	19940714

OS CASREACT 128:13139; MARPAT 128:13139

AB A 1-pot **synthesis** of sulfonamides from sulfones was developed. Conversion of sulfones to the corresponding sulfinic acid salts is followed by oxidative-amination to give the sulfonamides.

L37 ANSWER 11 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

reactions between $\text{Bu}_3\text{SnNMe}_2$ and aryl halides catalyzed by $\{\text{Pd}[\text{P}(\text{o-Tol})_3]_2\}$ (1), $\{\text{Pd}[\text{P}(\text{o-Tol})_3](\text{p-MeC}_6\text{H}_4)\text{Br}\}_2$ (2a), and $\{\text{Pd}[\text{P}(\text{o-Tol})_3](\text{NHMe}_2)(\text{p-MeC}_6\text{H}_4)\text{Br}\}$ (3a). A combination of kinetic studies and independent **synthesis** of reaction intermediates indicated that the three-coordinate Pt-group amido complex $\{\text{Pd}[\text{P}(\text{o-Tol})_3](\text{Ar})(\text{NMe}_2)\}$ was an intermediate in these reactions. Thus, these aryl halide aminations are rare examples of catalysis with a Pt-group amido complex. Kinetic data were obtained by ^1H NMR spectroscopy, and the rate behavior is zero order in added phosphine, zero order in aryl halide, and 1st order in Sn amide under conditions of equal or greater concns. of aryl bromide compared to Sn amide. Reactions catalyzed by 3a were 1st order in the Pd complex. Reaction rates were inhibited by added Sn bromide, but not by the arylamine product. The inhibition by Sn bromide showed that reversible transmetalation between an aryl halide complex and the Sn **reagent** was occurring. Subsequent to reversible transmetalation, a rate-detg. reductive elimination of arylamine occurred. Under conditions with a 10-fold excess of Sn amide and high phosphine concns., the rate-detg.-step became oxidative addn. of aryl bromide, and reactions became 1st order, rather than zero order, in aryl bromide. The amido intermediate deduced from kinetic studies appeared to be generated by reacting $\{\text{Pd}[\text{P}(\text{o-Tol})_3](\text{p-BuC}_6\text{H}_4)(\text{Br})\}_2$ with Li arylamides or by deprotonating $\{\text{Pd}[\text{P}(\text{o-Tol})_3](\text{NHMe}_2)(\text{p-BuC}_6\text{H}_4)(\text{Br})\}$ with $\text{MN}(\text{SiMe}_3)_2$ ($\text{M} = \text{K}, \text{Li}$). Both reactions gave yields of arylamine that were comparable to those of catalytic reactions. Competition and relative rate studies revealed an equil. between aryl halide complexes 2a-c and a Sn amide adduct of it. In competition studies involving an in situ selectivity for reaction of $\text{Bu}_3\text{SnNMe}_2$ or $\text{Bu}_3\text{SnNEt}_2$ with p-t-BuC₆H₄Br catalyzed by 1, the ratio of N,N-dimethylaniline to N,N-diethylaniline was 2.9. However, kinetic measurements of individual reactions showed that $\text{Bu}_3\text{SnNMe}_2$ reacted only 1.4 times faster than $\text{Bu}_3\text{SnNEt}_2$, consistent with a reversible equil. involving Sn amide binding to the catalyst, similar to that resulting from substrate binding preequil. in enzyme systems.

L37 ANSWER 13 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1995:579020 CAPLUS

DN 123:112190

TI **Synthesis** and Solid-State Structure of Substituted Arylphosphine Oxides

AU Whitaker, Craig M.; Kott, Kevin L.; McMahon, Robert J.

CS Department of Chemistry, University of Wisconsin, Madison, WI, 53706-1396, USA

SO Journal of Organic Chemistry (1995), 60(11), 3499-508

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

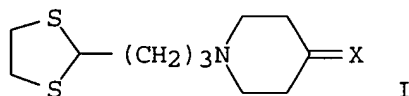
LA English

OS CASREACT 123:112190

AB The prepn. and characterization of several new arylphosphine oxides, which are of interest as second-order nonlinear optical materials is described. (4-Aminophenyl)diphenylphosphine oxide (1a), bis(4-aminophenyl)phenylphosphine oxide (2a), and (4-aminophenyl)bis[4'-(trifluoromethyl)phenyl]phosphine oxide (5) were prepd. by addn. of aryl Grignard and organolithium **reagents** contg. protected amines to phosphorus oxyhalides. Alternatively, 1a was prepd. by treatment of (4-bromophenyl)diphenylphosphine oxide with azidomethyl Ph sulfide, followed by hydrolysis. (4-Aminophenyl)(4'-nitrophenyl)phenylphosphine oxide (6) was prepd. by nucleophilic arom. substitution of bis(4-fluorophenyl)phenylphosphine oxide to give the corresponding

dinitro compd., followed by selective monoredn. The x-ray crystal structure of (4-aminophenyl)diphenylphosphine oxide (1a), along with those of mono-, di-, and trihydroxy triphenylphosphine oxides exhibit extensive intermol. hydrogen bonding. The hydrogen bonding in 1a and 1b produces chains of arylphosphine oxide mols. with a head-to-tail alignment; the chains pack in an antiparallel manner to produce solid-state structures that display only slight deviations from centrosymmetry.

L37 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1994:134337 CAPLUS
 DN 120:134337
 TI **Synthesis** of haloperidol ethanedithioketal HIV-1 protease inhibitors: magnesium chloride facilitated addition of Grignard **reagents**
 AU Sui, Zhihua; De Voss, James J.; DeCamp, Dianne L.; Li, Jia; Craik, Charles S.; Ortiz de Montellano, Paul R.
 CS Dep. Pharm. Chem., Univ. California, San Francisco, CA, 94143-0446, USA
 SO Synthesis (1993), (8), 803-8
 CODEN: SYNTBF; ISSN: 0039-7881
 DT Journal
 LA English
 GI



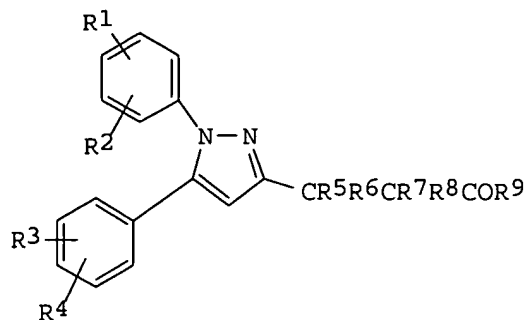
AB Haloperidol ketals and ethanedithioketals, e.g. I (X = O, OCH₂CH₂O), of interest as HIV-1 protease inhibitors were synthesized by addn. of organolithium and organomagnesium **reagents** to ketone precursors already contg. the ketal or thioketal functionality. Addn. of Grignard **reagents** to the thioketal contg. ketone was enhanced remarkably, and to the ketal contg. ketone moderately, by the addn. of magnesium chloride. The effect of magnesium chloride is attributed to its ability to competitively prevent chelation of the Grignard **reagent** and proton abstraction from the 4-oxopiperidine ring. The biol. activities of the ketals and thioketals indicate that the thioketal function conveys greater ability to inhibit the HIV-1 protease than the ketal function.

L37 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1990:590818 CAPLUS
 DN 113:190818
 TI Reaction of nitro compounds towards Grignard **reagents**. A general method of **synthesis** of N-alkyl- or N-aryl-N-propargylhydroxylamines
 AU Bartoli, Giuseppe; Palmieri, Gianni; Petrini, Marino; Bosco, Marcella; Dalpozzo, Renato
 CS Dip. Sci. Chim., Camerino, I-62032, Italy
 SO Gazzetta Chimica Italiana (1990), 120(4), 247-9
 CODEN: GCITA9; ISSN: 0016-5603
 DT Journal
 LA English
 OS CASREACT 113:190818
 AB Propargyl bromide was converted to the resp. allenylmagnesium bromide and

added to nitro compds. to give N-aryl-N-propargylhydroxylamines and N-alkyl-N-propargylhydroxylamines $\text{RN}(\text{CH}_2\text{C.tplbond.CH})\text{OH}$ I (R = Ph, 4-ClC₆H₄, 1-naphthyl, hexyl, cyclohexyl, 4-MeC₆H₄CH₂CH₂ etc.) in the presence of LiAlH₄ and Pd/C. I are not further reduced to give, e.g., N-propargylanilines.

L37 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1989:423508 CAPLUS
 DN 111:23508
 TI Antiinflammatory 2- and 3-substituted 3-(1',5'-diaryl-3'-pyrazolyl)propionic acid derivatives and their **synthesis**
 IN Murray, William V.; Wachter, Michael P.
 PA Ortho Pharmaceutical Corp., USA
 SO Eur. Pat. Appl., 47 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 293220	A2	19881130	EP 1988-304821	19880527
	EP 293220	A3	19900711		
	EP 293220	B1	19940831		
	R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
				US 1987-55806	19870529
				US 1988-181035	19880427
	AU 8816574	A1	19881201	AU 1988-16574	19880524
	AU 611437	B2	19910613		
				US 1987-55806	19870529
				US 1988-181035	19880427
	DK 8802899	A	19881130	DK 1988-2899	19880527
				US 1987-55806	19870529
				US 1988-181035	19880427
	JP 01052758	A2	19890228	JP 1988-128579	19880527
				US 1987-55806	19870529
				US 1988-181035	19880427
	ZA 8803831	A	19900131	ZA 1988-3831	19880527
				US 1987-55806	19870529
	CA 1319149	A1	19930615	CA 1988-567908	19880527
				US 1987-55806	19870529
				US 1988-181035	19880427
	ES 2058280	T3	19941101	ES 1988-304821	19880527
				US 1987-55806	19870529
				US 1988-181035	19880427
	US 5051518	A	19910924	US 1990-534325	19900604
				US 1987-55806	19870529
				US 1988-181035	19880427
	JP 09328475	A2	19971222	JP 1997-61724	19970303
	JP 2848375	B2	19990120		
				US 1987-55806	19870529
				US 1988-181035	19880427
				JP 1988-128579	19880527
OS	MARPAT 111:23508				
GI					



I

AB Title compds. I (R1-R4 = H, alkyl, alkoxy, H2N, H2NCO, Ph, halo, HO, alkylsulfonyl, alkylthio, NO2, F3C, .omega.-trifluoromethyl lower alkoxy; R1R2 or R3R4 together with the Ph to which they are attached, form a (substituted) naphthyl; R5-R8 = H, alkyl; R5-R8 = a part of a spirocycloalkyl, aryl, heterocyclyl; R6 and R8 together = part of a ring (cyclohexyl, cyclohexenyl, 7-oxobicyclo[2.2.1]heptenyl; R9 = HO, R10O, R10(HO)N; R10 = alkyl, etc.) useful in alleviating cardiovascular disorders (no data) and inflammation in mammals, are prepd. A NaH suspension in mineral oil and DMF was cooled to 0.degree. and PhCH2CO2Et in DMF was added dropwise and the resulting soln. stirred for 1 h followed by addn. of 3-bromomethyl-5-(4-chlorophenyl)-1-(4-methoxyphenyl)pyrazole (prepn. given) in DMF to give I (R1 = 4-MeO, R2, R3, R5, R6, R7 = H, R4 = 4-Cl, R8 = 4-ClPh, R9 = EtO) (II) in 45% yield. The antiinflammatory activity of II at 10 mg/kg in rats, expressed as percent inhibition of paw vol. increase was 61%.

=> d his

(FILE 'HOME' ENTERED AT 10:51:14 ON 21 NOV 2003)

FILE 'REGISTRY' ENTERED AT 10:51:20 ON 21 NOV 2003

L1 STRUCTURE UPLOADED

FILE 'CAPLUS' ENTERED AT 10:51:52 ON 21 NOV 2003

L2 172 S LITHIUM AND ARYL HALIDES
 L3 12 S LITHIUM AND FLUORO PHENYL
 L4 0 S PHENYL BORONIC ACID AND PHENYL BORINIS ACID
 L5 0 S PHENY BORONIC ACID
 L6 233 S PHENYL BORONIC ACID
 L7 3 S PHENYL BORINIC ACID
 L8 0 S L6 AND L7
 L9 0 S L3 AND L6
 L10 0 S L3 AND L2
 L11 1 S L2 AND PHENYL BORONIC ACID
 L12 0 S L2 AND PHENYL BORINIC ACID
 L13 1 S L2 AND L6
 L14 0 S L3 AND L6
 L15 1 S L2 AND L6
 L16 69 S PHENYL BORONIC ACID AND SYNTHESIS
 L17 2 S L16 AND LITHIUM
 L18 0 S SYNTHESIS AND PHENYL BORONIC ACID AND PRODUCTION
 L19 69 S SYNTHESIS AND PHENYL BORONIC ACID
 L20 3 S L19 AND ONE POT

L21 12 S LITHIUM AND PHENYL HALIDE
L22 172 S LITHIUM AND ARYL HALIDES
L23 0 S LITHIUM ARYL HALIDES
L24 0 S ARYL LITHIUM HALISE AND BORONIC ACIDS
L25 0 S ARYL LITHIUM HALIDES AND BORONIC ACIDS
L26 4 S L21 AND L22
L27 1118 S LITHIUM AND GRIGNARD REAGENT
L28 0 S L27 AND PHENYL BORONIC ACID
L29 0 S L27 AND PHENYL BORINIC ACID
L30 0 S PHENYL BORONIC ACID ANS SYNTHESIS
L31 69 S PHENYL BORONIC ACID AND SYNTHESIS
L32 0 S L31 AND L27
L33 0 S L31 AND LITIUM
L34 0 S L31 AND PHENYL LITHIUM FLUORIDE
L35 317 S LITHIUM AND FLUOROPHENYL
L36 90 S L35 AND SYNTHESIS
L37 16 S L36 AND REAGENT

=> s l27 and synthesis

L38 410 L27 AND SYNTHESIS

=> s l38 and phenyl boronic acid

L39 0 L38 AND PHENYL BORONIC ACID

=> s l39 and boronic acid

L40 0 L39 AND BORONIC ACID

=> s l39 and borinic acid

L41 0 L39 AND BORINIC ACID

=> s aryl lithium and halides

L42 5 ARYL LITHIUM AND HALIDES

=> s phenyl lithium and halides

L43 15 PHENYL LITHIUM AND HALIDES

=> s phenyl boronic acids

L44 6 PHENYL BORONIC ACIDS

=> s l43 and l44

L45 0 L43 AND L44

=> s l43 and synthesis

L46 2 L43 AND SYNTHESIS

=> d l46 fbib hitstr abs total

L46 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1997:347170 CAPLUS

DN 127:17742

TI **Synthesis** and Structures of Intramolecularly Base-Coordinated
Group 15 Aryl **Halides**

AU Carmalt, Claire J.; Cowley, Alan H.; Culp, Robert D.; Jones, Richard A.;
Kamepalli, Smuruthi; Norman, Nicholas C.

CS Department of Chemistry Biochemistry, University of Texas, Austin, TX,
78712, USA

SO Inorganic Chemistry (1997), 36(13), 2770-2776
CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society
DT Journal
LA English
AB Four group 15 monochlorides of the type EAr_2Cl [$\text{Ar} = 2$ -[(dimethylamino)methyl]phenyl, 2-(Me₂NCH₂)C₆H₄ (C₉H₁₂N), E = Sb (4), E = Bi (5); Ar = 8-(dimethylamino)-1-naphthyl, 8-(Me₂N)C₁₀H₆ (C₁₂H₁₂N), E = Sb (6), E = Bi (7)] have been prepd. via the salt elimination reactions of 2 equiv. of either 2-(Me₂NCH₂)C₆H₄Li or 8-(Me₂N)C₁₀H₆Li with ECl_3 . Four related group 15 dihalides of the type EAr_2X_2 [$\text{Ar} = 8$ -(Me₂N)C₁₀H₆, X = Cl, E = As, (8), E = Sb (9); Ar = 2-(Me₂NCH₂)C₆H₄, X = Cl, E = Bi (10); X = I, E = Bi (11)] have been prepd. via the salt elimination reactions of equimolar amts. of 8-(Me₂N)C₁₀H₆Li or 2-(Me₂NCH₂)C₆H₄Li with EX_3 . The x-ray crystal structures of 4-6, 8, 9, and 11 are described, and the obsd. trends in the degree of intramol. coordination of the nitrogen atoms are consistent with the view that the Lewis acidity of these complexes is assocd. with the E-X σ^* orbitals. Crystal data for 4: triclinic, space group P $\bar{1}$, $a = 9.1483(1)$.ANG., $b = 9.4868(1)$.ANG., $c = 12.9776(2)$.ANG., $\alpha = 70.614(8)$.degree., $\beta = 85.738(9)$.degree., $\gamma = 83.094(9)$.degree., $V = 1054.0(2)$.ANG.³, $Z = 2$, $R = 0.0420$. Crystal data for 5: monoclinic, space group P2₁/c, $a = 11.9498(1)$.ANG., $b = 11.4695(1)$.ANG., $c = 13.9456(8)$.ANG., $\beta = 104.536(6)$.degree., $V = 1850.2(3)$.ANG.³, $Z = 4$, $R = 0.0375$. Crystal data for 6: monoclinic, space group P2₁/n, $a = 9.4991(8)$.ANG., $b = 23.455(4)$.ANG., $c = 9.726(1)$.ANG., $\beta = 100.629(8)$.degree., $V = 2129.8(4)$.ANG.³, $Z = 4$, $R = 0.0406$. Crystal data for 8: orthorhombic, space group P2₁2₁2₁, $a = 9.713(3)$.ANG., $b = 9.835(4)$.ANG., $c = 13.310(3)$.ANG., $V = 1273.8(5)$.ANG.³, $Z = 4$, $R = 0.0695$. Crystal data for 9: orthorhombic, space group P2₁2₁2₁, $a = 9.7140(3)$.ANG., $b = 10.0196(1)$.ANG., $c = 13.444(3)$.ANG., $V = 1308.5(3)$.ANG.³, $Z = 4$, $R = 0.0320$. Crystal data for 11: monoclinic, space group P2₁/c, $a = 7.9455(7)$.ANG., $b = 19.3949(3)$.ANG., $c = 8.6226(9)$.ANG., $\beta = 93.338(9)$.degree., $V = 1326.5(2)$.ANG.³, $Z = 4$, $R = 0.0379$.

L46 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:479406 CAPLUS
DN 125:221917
TI Isolation and Reduction of Sterically Encumbered Arylboron Dihalides: Novel Boranediyl Insertion into C-C σ -Bonds
AU Grigsby, Warren J.; Power, Philip P.
CS Department of Chemistry, University of California, Davis, CA, 95616, USA
SO Journal of the American Chemical Society (1996), 118(34), 7981-7988
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 125:221917
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The **synthesis** and subsequent redn. of the arylboron dihalides 2,6-Mes₂C₆H₃ BX₂ (X = Cl (1); Br (2)) and 2,6-Trip₂C₆H₃ BBr₂ (3) (Mes = 2,4,6-Me₃C₆H₂- and Trip = 2,4,6-i-Pr₃C₆H₂-) are described. Treatment of 2 with Li metal in Et₂O gave the novel Li 9-borafluorenyl compds. 4 (shown as I) and 5 (shown as II) in which the boranediyl intermediate has

inserted into an o-Me-ring C-C .sigma.-bond to form a borafluorenyl structure incorporating B in a delocalized five-membered ring. Boranediyl insertion into C-C .sigma.-bonds, as distinct from boranediyl induced rearrangements involving C:C cleavage in delocalized arom. substrates, is unknown. The main difference between the structures of these products is that 5 is dimerized as a consequence of the redn. in the no. of solvating ethers. Redn. of 2 with KC8 gave the 9-borafluorenyl ate compds. 6 and 7 (shown as III; L = THF, C6H6). These products also result from C-C bond insertion by B as seen in 4 and 5. However, the delocalization is not obsd. owing to the addn. of H (presumably from solvent) to the borons affording borate salts. Redn. of 3 with 3 equiv of KC8 furnishes the new diborate species 8 (shown as IV). This compd. features as unique B-B bonded dianionic structure with a long (1.83(2) .ANG.) B-B bond which arises from the assocn. of two borate radical anion fragments that have a 9-borafluorenyl structure similar to those described above. 2-8 Were characterized by 1H, 13C, 7Li, and 11B NMR spectroscopy and by x-ray crystallog.

=> d his

(FILE 'HOME' ENTERED AT 10:51:14 ON 21 NOV 2003)

FILE 'REGISTRY' ENTERED AT 10:51:20 ON 21 NOV 2003

L1 STRUCTURE UPLOADED

FILE 'CAPLUS' ENTERED AT 10:51:52 ON 21 NOV 2003

L2 172 S LITHIUM AND ARYL HALIDES
 L3 12 S LITHIUM AND FLUORO PHENYL
 L4 0 S PHENYL BORONIC ACID AND PHENYL BORINIS ACID
 L5 0 S PHENY BORONIC ACID
 L6 233 S PHENYL BORONIC ACID
 L7 3 S PHENYL BORINIC ACID
 L8 0 S L6 AND L7
 L9 0 S L3 AND L6
 L10 0 S L3 AND L2
 L11 1 S L2 AND PHENYL BORONIC ACID
 L12 0 S L2 AND PHENYL BORINIC ACID
 L13 1 S L2 AND L6
 L14 0 S L3 AND L6
 L15 1 S L2 AND L6
 L16 69 S PHENYL BORONIC ACID AND SYNTHESIS
 L17 2 S L16 AND LITHIUM
 L18 0 S SYNTHESIS AND PHENYL BORONIC ACID AND PRODUCTION
 L19 69 S SYNTHESIS AND PHENYL BORONIC ACID
 L20 3 S L19 AND ONE POT
 L21 12 S LITHIUM AND PHENYL HALIDE
 L22 172 S LITHIUM AND ARYL HALIDES
 L23 0 S LITHIUM ARYL HALIDES
 L24 0 S ARYL LITHIUM HALISE AND BORONIC ACIDS
 L25 0 S ARYL LITHIUM HALIDES AND BORONIC ACIDS
 L26 4 S L21 AND L22
 L27 1118 S LITHIUM AND GRIGNARD REAGENT
 L28 0 S L27 AND PHENYL BORONIC ACID
 L29 0 S L27 AND PHENYL BORINIC ACID
 L30 0 S PHENYL BORONIC ACID ANS SYNTHESIS
 L31 69 S PHENYL BORONIC ACID AND SYNTHESIS
 L32 0 S L31 AND L27

L33 0 S L31 AND LITHIUM
L34 0 S L31 AND PHENYL LITHIUM FLUORIDE
L35 317 S LITHIUM AND FLUOROPHENYL
L36 90 S L35 AND SYNTHESIS
L37 16 S L36 AND REAGENT
L38 410 S L27 AND SYNTHESIS
L39 0 S L38 AND PHENYL BORONIC ACID
L40 0 S L39 AND BORONIC ACID
L41 0 S L39 AND BORINIC ACID
L42 5 S ARYL LITHIUM AND HALIDES
L43 15 S PHENYL LITHIUM AND HALIDES
L44 6 S PHENYL BORONIC ACIDS
L45 0 S L43 AND L44
L46 2 S L43 AND SYNTHESIS

=> d l44 fbib hitstr abs total

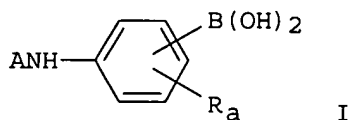
L44 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2003:253273 CAPLUS
DN 139:164822
TI Design and synthesis of **phenyl boronic acids**
and benzothiophenones as anticholinesterases
AU Lee, Eun Seok; Choi, Byoung Wook; Jung, Dai Il; Hwang, Hye Jung; Hahn,
Jung Tae; Lee, Bong Ho
CS Department of Chemical Technology, Hanbat National University, Daejeon,
305-719, S. Korea
SO Bulletin of the Korean Chemical Society (2003), 24(2), 243-245
CODEN: BKCSDE; ISSN: 0253-2964
PB Korean Chemical Society
DT Journal
LA English
AB Ph boronic acids, I- Me₃N+C₆H₃B(OCH₂CH₂O)-3 (1) and I- Me₃N+C₆H₃B(OH)₂-3
(2), were prepd. from methylation (MeI/MeOH/K₂CO₃) of 3-aminophenyl-1-boro-
2,5-dioxolane (for 1) and acid hydrolysis of 1 (for 2) and their
anticholinesterase activity tested. 3(H)benzothiophen-1-one and its
4-nitro deriv. were prepd. from reaction of methylbenzoate reaction with
benzoylperoxide/N-bromosuccinimide and thiourea and their
anticholinesterase activity tested.
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L44 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:542707 CAPLUS
TI Synthesis of TEG-linked **phenyl boronic acids**
and their binding to saccharides.
AU Frisby, Xenia Yvette; Gervay, Jacquelyn
CS Department of Chemistry, University of Arizona, Tucson, 85721, USA
SO Book of Abstracts, 218th ACS National Meeting, New Orleans, Aug. 22-26
(1999), ORGN-326 Publisher: American Chemical Society, Washington, D. C.
CODEN: 67ZJA5
DT Conference; Meeting Abstract
LA English
AB A tri(ethylene) glycol (TEG) diphenylboronic acid deriv. was synthesized
as a substrate for binding lactose. An NMR study was conducted to observe
the binding capacity of the TEG deriv. to lactose as opposed to other
sugars. This NMR study was done as a model to det. the possible binding
affinity of a polymeric substrate that is to be used as a solid phase
filter for the extn. of lactose from soln.

L44 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1998:600340 CAPLUS
 DN 129:343321
 TI A general chemoenzymic synthesis of enantiopure cis .beta.-amino alcohols from microbially derived cis-glycols
 AU Lakshman, Mahesh K.; Chaturvedi, Surendrakumar; Zajc, Barbara; Gibson, David T.; Resnick, Sol M.
 CS Chemsyn Science Laboratories, Lenexa, KS, 66215, USA
 SO Synthesis (1998), (9), 1352-1356
 CODEN: SYNTBF; ISSN: 0039-7881
 PB Georg Thieme Verlag
 DT Journal
 LA English
 OS CASREACT 129:343321
 AB Enantiomerically pure cis-glycols, derived through the microbial metab. of hydrocarbons, represent a valuable chiral pool for the synthesis of cis .beta.-amino alcs. A generally applicable route to these important chiral intermediates is described. Reaction of the metabolically formed diol with AcOCMe₂COCl affords regio- and stereoselectively a single trans-1,2-chlorohydrin acetate isomer. Displacement of Cl by N₃, aminolysis of the ester, and redn. of the azide provides the requisite amino alcs. This 4-step route is highly efficient and affords the cis .beta.-amino alc. enantiomers in 41-57% overall yield. Using the highly enantiopure amino alcs., diastereomeric oxazaborolidines were prepd. with both (-)-(S)- and (+)-(R)-[2-(1-methoxyethyl)**phenyl**]**boronic acids**. As described herein, these derivs. are potentially useful for abs. configurational assignments to cis amino alcs.

L44 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1996:197250 CAPLUS
 DN 124:289871
 TI Phenylboronic acid derivatives for introduction of boronic acid group and their preparation
 IN Waki, Kazunori; Shiino, Taijiro; Sakurai, Yasuhisa; Okano, Mitsuo; Kataoka, Kazunori; Koyama, Yoshuki; Ishihara, Shoji
 PA Nippon Oils & Fats Co Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 10 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

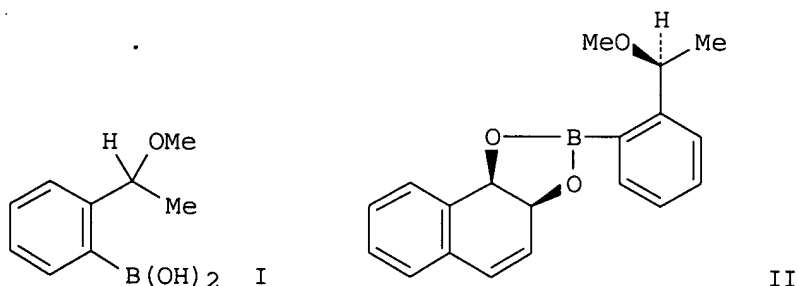
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 08003172	A2	19960109	JP 1994-133290	19940615
				JP 1994-133290	19940615
OS	MARPAT 124:289871				
GI					



AB The derivs. I [A = COCHR₁(CH₂)_nNH₂; R = F, CbF₂bX (X = F, H, Cl; b =

1-10), $\text{CF}(\text{CF}_3)[\text{OCF}_2\text{CF}(\text{CF}_3)]\text{COC}_3\text{F}_7$ ($c = 0-8$); $\text{R}_1 = \text{H}$, C_1-10 hydrocarbyl; $n = 0-6$) (II) are prepd. by treatment of I ($A = \text{H}$) with amino-protected amino acids followed by deprotection. The aminoalkyl group effectively reacts with polymers and drugs, the boronic acid group is capable of forming reversible complexes with OH group of sugars, and fluoroalkyl group is electron-attractive, therefor II are useful for synthesis of functional compds. A THF soln. of 0.638 g Z-Gly was treated with carbonyldiimidazole at 0.degree. for 90 min and the reaction mixt. was further treated with 0.254 g 3-amino-6-(heptafluoropropyl)phenylboronic acid (adduct with EtOH) at room temp. for 50 h to give 72% amide. The amide (250 mg) was reduced in the presence of Pd/C to give 46 mg 3-aminoacetyl amino-6-(heptafluoropropyl)phenylboronic acid (III). A DMF soln. of III and Et₃N was treated with N-vinylpyrrolidone-maleic anhydride copolymer at 40.degree. for 24 h and the polymer obtained was treated with an aq. NaHCO₃ at 60.degree. for 3 h to open the unreacted anhydride ring to give a polymer having phenylboronic acid group at 100% reaction rate.

L44 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1995:578967 CAPLUS
 DN 123:198391
 TI Chemoenzymic Synthesis of Chiral Boronates for the Determination of the Absolute Configuration and Enantiomeric Excess of Bacterial and Synthetic cis-Dienediols
 AU Resnick, Sol M.; Torok, Daniel S.; Gibson, David T.
 CS Department of Microbiology, University of Iowa, Iowa City, IA, 52240, USA
 SO Journal of Organic Chemistry (1995), 60(11), 3546-9
 CODEN: JOCEAH; ISSN: 0022-3263
 PB American Chemical Society
 DT Journal
 LA English
 GI



AB A chemoenzymic, divergent synthesis is was described for producing enantiomerically pure 2-[1-methoxyethyl]phenyl boronic acids (I) which serve as reagents in a procedure for ¹H NMR detn. of abs. configuration and enantiomeric excess of cis-diene diols formed by the bacterial dioxygenation of mono- and polycyclic arenes. Consistent trends (¹H NMR directional shifts) are reported for the diastereomeric OMe and Me signals of boronate esters formed with (+)- and (-)-I, and homochiral cis-diene diols (of known configuration) obtained by the bacterial dioxygenation of toluene, trifluoromethyltoluene, biphenyl, naphthalene, dihydronaphthalene, anthracene, and biphenylene. The formation of Diels-Alder cycloadducts (via 4-phenyl-1,2,4-triazoline-3,5-dione) prior to derivatization with (+)-I and (-)-I allowed application of

the methodol. for the cis-halocyclohexadiene diols. The method is simple, applicable to small sample amts. (<2 mg), requires little or no purifn. of products prior to NMR anal., and can be used to det. abs. configuration and enantiomeric excess of bacterial and synthetic cis-diene diols. The example compd. II was prepd. from (1R-cis)-1,2-dihydro-1,2-naphthalenediol.

L44 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1956:67889 CAPLUS

DN 50:67889

OREF 50:12609d-e

TI Stability, solvolysis, and coordination reactions of esters of boronic acids and their halogen derivatives

AU Brindley, P. B.; Gerrard, W.; Lappert, M. F.

CS Northern Polytech., London

SO Journal of the Chemical Society, Abstracts (1956) 1540-5

CODEN: JCSAAZ; ISSN: 0590-9791

DT Journal

LA Unavailable

AB The esters and haloesters of butyl and **phenyl boronic acids** and of butyl and phenyl boron dihalides were studied. The thermal stability, hydrolysis, alcoholysis, and coordination (with pyridine) are discussed. Possible mechanisms are given and the similarity of the reactions of these compds. to those of the borates, alkoxyboron halides, and boron trihalides is described.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

273.26

273.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-19.53

-19.53

STN INTERNATIONAL LOGOFF AT 11:15:02 ON 21 NOV 2003